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EFFECT OF TEMPERATURE FIELD ON COAL DEVOLATILIZATION IN A MILLISECOND DOWNER REACTOR

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ABSTRACT

A comprehensive CFD-DPM model was established to describe coal pyrolysis in millisecond downer reactors under high temperatures. The model predictions revealed the fact that the reactor performance is dominated by the design of the temperature field to guarantee fast, sufficient heating of coal particles in milliseconds.

INTRODUCTION

Coal pyrolysis to acetylene in thermal plasma provides a direct route to make chemicals from coal resources (1-3). Since the coal pyrolysis process is accommodated in a multiphase downer reactor operated under extreme conditions (e.g., an ultra-high temperature greater than 3000 K), multiple physical and chemical processes are completed in milliseconds of contact time, where the rapid heating and release of volatile matter in coal particles play the dominant role in the overall reactor performance. It has been acknowledged that thermal energy is the driving force for coal devolatilization. Therefore, the reactor design is actually directed to the appropriate design of the temperature field inside the reactor to guarantee sufficiently, fast heating of coal particles in milliseconds.

A comprehensive computational fluid dynamics model with a discrete phase model (CFD-DPM) was developed to understand the complex gas-particle reaction behavior in the coal pyrolysis millisecond process. The model incorporated particle-scale physics such as heat conduction inside solid materials, diffusion of released volatile gases (4), coal devolatilization, and the tar cracking reaction (5-6). The chemical percolation devolatilization (CPD) model (7-9) was applied to describe the devolatilization behavior of rapidly heated coal based on the physical and chemical transformations of the coal structure. The predictions by the CFD-DPM method were validated by comparing the predicted volume fractions of the main species and light gas yields with the experimental data under a set of typical operating conditions from the 5-MW coal pyrolysis plasma reactor (10). The results showed that the heating histories and the devolatilization of particles with the same diameter were mainly determined by the surrounding temperature field. That is to say, different heating histories experienced by the particle led to different heating rates as well as the heating time of the particles, and different yields of light gases.

For further illustration of the effect of the temperature field on the heating histories of particles and coal devolatilization, different reactor designs were modeled using CFD-DPM. The same energy input to the downer reactor was assumed by fixing the pre-defined enthalpy streams of gases, the heat input through the reactor wall, and the coal feeding conditions. The results showed that coal particles exhibited different devolatilization performance when experiencing different temperature histories. Accordingly, reactor optimization can be determined with the guidance of the above simulation.

MODEL DESCRIPTION

The comprehensive CFD-DPM model includes the *k-ε* turbulence model for gaseous turbulent flow with heat and mass transfer, the mixture fraction approach with the probability density function (PDF) method of modeling the interaction of turbulence and chemistry, the chemical equilibrium model for high temperature gas-phase chemical reactions, the discrete phase model (DPM) for momentum, heat and mass transfer between gas and particles and sub-models for the devolatilization of coal particles.

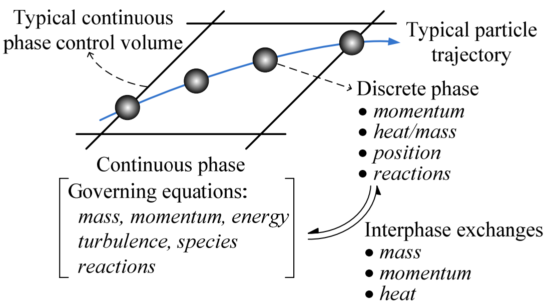

Figure 1 Heat, mass and momentum transfer between the discrete and continuous phases

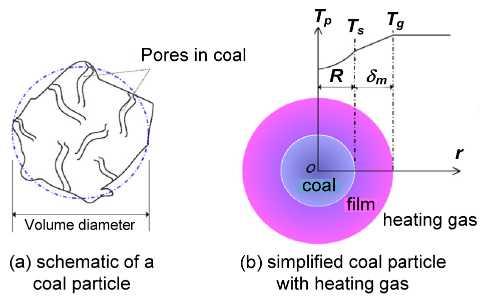

Figure 2 Schematic of a coal particle with heating gas

The numerical simulations of gas-particle flows follow the Eulerian-Lagrangian approach, as shown in Figure 1. The fluid phase is treated as a continuum by solving the Navier-Stokes equations, while the particle is considered as the dispersed phase, solved by tracking a large number of particles through the calculated flow field. As the trajectory of each particle is computed, the momentum, mass and energy exchange between the particles and the continuous phase is added to the source term of the discretization equations for the gas continuum (see Chen and Cheng (11)).

In addition, the heat transfer model inside a particle (as shown in Figure 2) is established based on the conduction equation with consideration of the heat of pyrolysis and the heat conduction in solid materials:

$$\left(\rho c_p\right)_{eff} \frac{\partial T(r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda_{eff} r^2 \frac{\partial T(r,t)}{\partial r}\right) - \Delta_r H \cdot \gamma_{vol}(r,t) \tag{1}$$

where

$$\left(\rho c_p\right)_{eff} = \varepsilon \rho_{vol} c_{p,vol} + \left(1-\varepsilon\right)\rho_p c_{p,p} \tag{2}$$

$$\lambda_{eff} = \varepsilon \lambda_{vol} + \left(1-\varepsilon\right)\lambda_p \tag{3}$$

In these equations, $T(r,t)$ represents the local temperature at any radial position r and time t, ε is the porosity of particle; ρ_p and ρ_{vol} are the densities of the solid material and the volatile phases, respectively; $c_{p,p}$ and $c_{p,vol}$ are the specific heat capacities of the solid material and volatile phases, respectively; λ_{eff} is the effective local thermal conductivity; λ_p and λ_{vol} represent the thermal conductivities of the solid material and volatile phases, respectively; $\Delta_r H$ is the heat of pyrolysis; and $\gamma_{vol}(r,t)$ denotes the rate of devolatilization ($kg/m^3 \cdot s$).The boundary conditions of Eq. (1) are given as:

$$\begin{cases} 4\pi R^2 \lambda_{eff} \left.\dfrac{\partial T}{\partial r}\right|_{r=R} = 4\pi\left(R+\dfrac{\delta_m}{2}\right)^2 h\left(T_g - T_w\right)\theta + \sigma\varepsilon_p (4\pi R^2)\left(T_g^4 - T_w^4\right) \\ \left.\dfrac{\partial T}{\partial r}\right|_{r=0} = 0 \end{cases} \tag{4}$$

where R is the radius of the coal particle, T_w is the temperature at the surface of the coal particle, T_g is the local temperature of the continuous phase, σ is the Stefan-Boltzmann constant, ε_p is the black-body radiation coefficient for the pulverized coal, δ_m is the thickness of the gas film around the coal particle (estimated to be $2R$ at a relative small Reynolds number in this study), h is the gas-particle heat transfer coefficient, and θ is a factor related to the effect of volatiles' release on heat conduction. The gas-particle heat transfer coefficient was calculated from the Nusselt number, $Nu = h\delta_m/\lambda_m$, where λ_m is the thermal conductivity of the gas film. The factor θ reported by Spalding (12) was adopted in this study,

$$\theta = \frac{B}{e^B - 1},\ B = \frac{c_{\mathrm{p,g}}}{2\pi d_{\mathrm{p}} \lambda_{\mathrm{m}}}\left(\frac{dm_{\mathrm{vol}}}{dt}\right) \tag{5}$$

where $c_{\mathrm{p,g}}$ represents the gas specific heat capacity, d_{p} is the particle diameter, *and* dm_{vol}/dt denotes the formation rate of volatiles from coal (kg/s).

The CPD model was employed to describe the devolatilization of coal particles, where the fractional change in the coal mass as a function of time was divided into light gases, tar precursor fragments and char. The tar cracked through the following assumed paths:

$$light\ gases \xleftarrow{k_1} Tar \xrightarrow{k_2} soot \tag{6}$$

The mechanism utilizes the Arrhenius equation which is defined as:

$$k_i = A_i \exp\left(-E_i / RT\right) \qquad i = 1,2 \tag{7}$$

The values of the kinetic parameters were obtained from the work of Ma (5) and Brown (6).

The solution of the complex model described above was implemented using the commercial software FLUENT with self-developed user-defined functions (UDFs).

RESULTS AND DISCUSSION

Model validation

Figure 3 shows a schematic drawing of the 5-MW plasma downer reactor for coal pyrolysis, which was composed of the V-shaped plasma torch, the mixing zone, the reaction zone and the quench and separator.

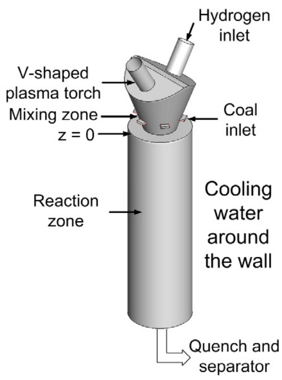

Figure 3 Schematic drawing of the 5-MW plasma downer reactor

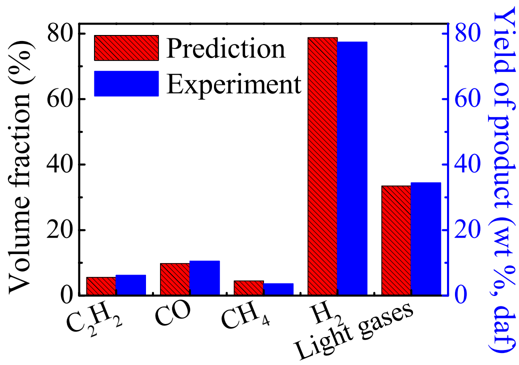

Figure 4 Comparison of predictions with the experimental data of the 5-MW reactor

The predicted volume fractions of the main species and the yield of light gases using this practical geometry are plotted in Figure 4, together with typical experimental data. The predictions and the actual performance of the 5-MW pilot reactor are based on typical operating conditions (10). It can be seen from Figure 4 that the model predictions agreed well with the experimental data. Therefore, the comprehensive CFD-DPM model is qualified for describing the complex devolatilization process in the reactor under the extreme environmental conditions such as ultrahigh temperatures and the milliseconds reaction time. Meanwhile, the simulations can help to optimize the operating conditions and improve reactor performance.

Reaction process of coal particles

Figure 5 shows the variations of the particle temperature and yields of light gases with particle residence time in the 5-MW downer reactor, together with the temperature of the heating gas around the particle trajectories. The unique structure of V-shaped torch causes the uniform temperature distribution and the corresponding uniform velocity field in the reactor. Therefore, Coal particles with a diameter of 50 μm injected from different positions experience different heating histories, which result in different devolatilization performances. It can be shown that the effect of the surrounding temperature field on the particle heating history and devolatiliation performance is significant.

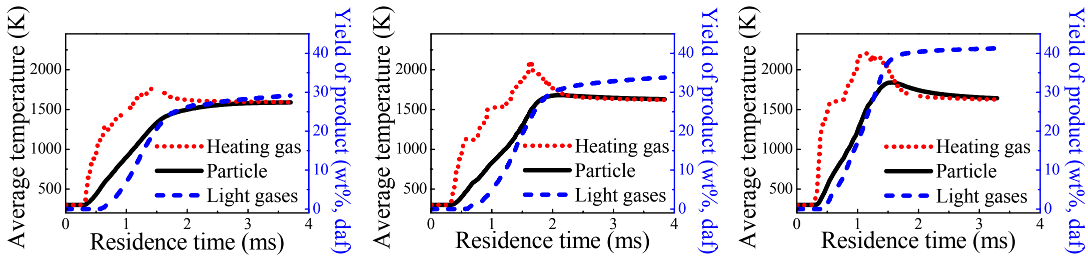

Figure 5 Reaction process of a single representative particle in the 5-MW downer reactor

Effect of the specified temperature field

For further illustration of the effect of temperature field on the particle heating history and devolatilization performance, variations of the particle temperature and devolatilization versus the particle residence time under different specified temperature fields are plotted in Figure 6. It is assumed that coal particles with a diameter of 50 μm passed through the preset temperature field and the temperature of the heating gas was not impacted by the discrete particles.

When the particle residence time is long enough to ensure that the temperature of the particle is close to that of the heating gas, a higher surrounding temperature would lead to a faster heating rate, and therefore a better devolatilization performance. The devolatilization is almost competed once the particle reaches its peak temperature. After that, thermal energy is no longer the main driving force for the coal devolatilization process. Therefore, in order to get a better devolatilization performance and a higher energy utilization efficiency, the thermal energy should be used for maintaining a high temperature field to make sure the coal particle is heated to a higher temperature.

When the surrounding temperature field is fixed, the particle heating histories and yields of light gases are observed to be very sensitive to changes in the heat up time, as shown in Figure 7. The optimal residence time in the high temperature zone should be more than 2 ms under this situation. When the heat up time is less than 1 ms, the thermal energy stored in the high temperature heating gas was not used effectively to achieve satisfactory reactor performance.

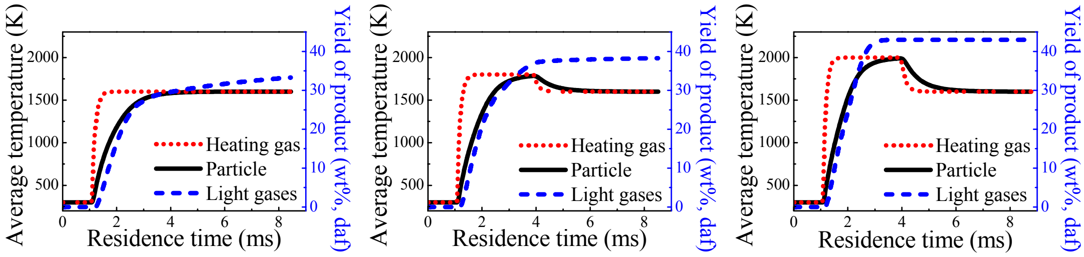

Figure 6 Effect of temperature field on particle heating history and devolatilization performance

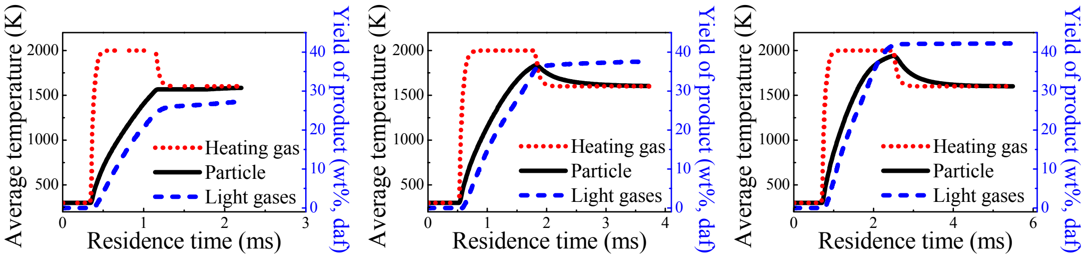

Figure 7 Effect of heating time on the particle heating history and devolatilization performance

Effect of reactor design

The reactor design is actually directed to the design of the temperature field inside the reactor, as shown in Figure 8. Three kinds of energy input designs are carried out to investigate the influences of reactor design on the particle heating history and the yield of light gases. The feed conditions to the downer reactors are fixed and the same amount of energy is exerted into the different specified reactor wall,

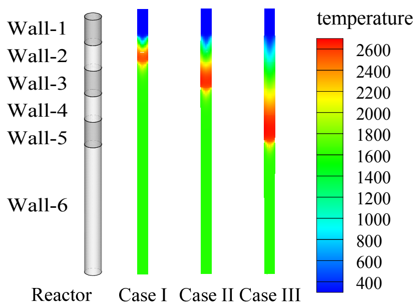

Figure 8 Temperature field of different reactors

i) Case I: all the energy is inputted to the reactor only through wall-2;

ii) Case II: all the energy is inputted to the reactor through wall-2 and wall-3 evenly;

iii) Case III: all the energy is inputted to the reactor through wall-2, wall-3, wall-4 and wal-5 evenly;

The temperature of wall-1 is fixed at 300K and the ones of other walls are fixed at 1600 K for all cases. The input energy density of each reactor design is: Case I, 1.4e6 W/m^2; Case II, 7e5 W/m^2; Case III, 3.5e5 W/m^2. It is shown in Figure 8 that different reactor designs cause different temperature fields, which leads to a different devolatilization performance. Too concentrated an energy input (e.g., Case I) leads to a shorter heat up time as well as a lower peak temperature of the coal particle. As a result, a poor devolztilization performance is obtained. The appropriate energy input density is achieved when both a high temperature field and enough heat up time occurs, which leads to the higher yield of light gases, as shown in Figure 9.

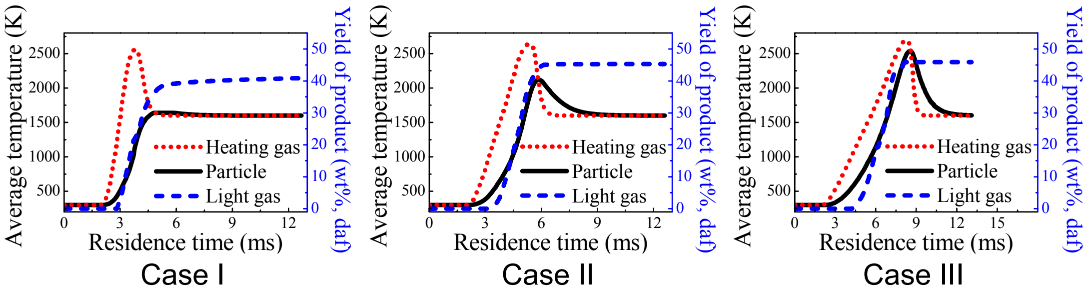

Figure 9 Effect of reactor design on the particle heating history and devolatilization performance

The temperature field can be designed by altering the operating conditions. In order to get a better devolatilization performance, special attention must be paid to the design of the high-temperature heat source and the gas-particle mixing efficiency to ensure that the coal particles can be heated up rapidly have sufficient time in the high temperature zone.

CONCLUSION

A comprehensive CFD-DPM model was established to describe coal devolatilization in millisecond downer reactors with successful validation using experimental data. This model was further employed to explore the effect of temperature field on the particle heating history and devolatilization performance. The results indicate that the coal particles exhibit different devolatilization performances when experiencing different designed temperature histories. Faster heat up rates, higher gas temperatures and longer residence times lead to a better devolatilization performance. With the guidance of these simulations, the reactor design and operating conditions can be selected to obtain the best temperature field and excellent gas-particle mixing efficiency in order to achieve a better reactor performance.

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REFERENCES

1. Bond, R. L., Ladner, W. R., Mcconnell, G. I. T., and Galbraith, I. F. (1963). "Production of Acetylene from Coal, Using a Plasma Jet." *Nature*, 200(491), 1313-1314.
2. Nicholso, R., and Littlewo, K. (1972). "Plasma Pyrolysis of Coal." *Nature*, 236(5347), 397-400.
3. Fauchais, P., Bourdin, E., Aubreton, J., and Amouroux, J. (1980). "Plasma Chemistry and Its Applications to The Synthesis of Acetylene from Hydrocarbons and Coal." *Int. Chem. Eng*, 20(2), 289-305.
4. Shuang, Y., Wu, C. N., Yan, B. H., and Cheng, Y. (2010). "Heat Transfer inside Particles and Devolatilization for Coal Pyrolysis to Acetylene at Ultrahigh Temperatures." *Energy & Fuels*, 24(5), 2991-2998.
5. Ma, J. (1996). "Soot Formation and Soot Secondary Reactions During Coal Pyrolysis." *PhD thesis, Brigham Young University, Utah, USA*.
6. Brown, A. L. (1997). "Modeling Soot in Pulverized Coal Flames." *MSc thesis, Brigham Young University, Utah, USA.*
7. Grant, D. M., Pugmire, R. J., Fletcher, T. H., and Kerstein, A. R. (1989). "Chemical Model of Coal Devolatilization Using Percolation Lattice Statistics." *Energy & Fuels*, 3(2), 175-186.
8. Fletcher, T. H., Kerstein, A. R., Pugmire, R. J., and Grant, D. M. (1990). "Chemical Percolation Model for Devolatilization. 2. Temperature and Heating Rate Effects on Product Yields." *Energy & Fuels*, 4(1), 54-60.
9. Fletcher, T. H., Kerstein, A. R., Pugmire, R. J., Solum, M. S., and Grant, D. M. (1992). "Chemical Percolation Model for Devolatilization. 3. Direct Use of C-13 Nmr Data to Predict Effects of Coal Type." *Energy & Fuels,* 6(4), 414-431.
10. Yan, B.H., Wu, C.N., Jin, Y., & Cheng, Y. (2010, May). "CFD simulation of the reacting flow process of coal pyrolysis to acetylene in hydrogen plasma downer reactors." In S.D. Kim, Y. Kang, J.K. Lee, & Seo, Y.C. (Eds.), *Fluidization XIII* (p.725), Engineering Conferences International, Gyeong-ju, Korea.
11. Chen, J. Q., and Cheng, Y. (2009). "Process Development and Reactor Analysis of Coal Pyrolysis to Acetylene in Hydrogen Plasma Reactor." *J. Chem. Eng. JPN*, 42, s103-s110.
12. Spalding, D. B. (1955). "Some Fundamentals of Combustion." *Butterworths Scientific Publications: London*.